On contact numbers of totally separable unit sphere packings *

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Abstract

Contact numbers are natural extensions of kissing numbers. In this paper we give estimates for the number of contacts in a totally separable packing of n unit balls in Euclidean d-space for all $n > 1$ and $d > 1$.

1 Introduction

Let $\mathbb{E}^d$ denote d-dimensional Euclidean space. Then the *contact graph* of an arbitrary finite packing of unit balls (i.e., of an arbitrary finite family of closed balls having unit radii and pairwise disjoint interiors) in $\mathbb{E}^d$ is the (simple) graph whose vertices correspond to the packing elements and whose two vertices are connected by an edge if and only if the corresponding two packing elements touch each other. The number of edges of a contact graph is called the *contact number* of the given unit ball packing. One of the most basic questions on contact graphs is to find the maximum number of edges that a contact graph of a packing of n unit balls can have in $\mathbb{E}^d$. Harborth [15] proved the following optimal result in $\mathbb{E}^2$: the maximum contact number of a packing of n unit disks in $\mathbb{E}^2$ is $\lfloor 3n - \sqrt{12n-3} \rfloor$, where$\lfloor \cdot \rfloor$ denotes the lower integer part of the given real. In dimensions three and higher the following upper bounds are known for the maximum contact numbers. It was proved in [9] that the contact number of an arbitrary packing of n unit balls in $\mathbb{E}^3$ is always less than $6n - 0.926n^{\frac{2}{3}}$. On the other hand, it is proved in [6] that for $d \geq 4$ the contact number of an arbitrary packing of n unit balls in $\mathbb{E}^d$ is less than $\frac{1}{2}\tau_d\, n - \frac{1}{2^d}\delta_d^{-\frac{d-1}{d}}\; n^{\frac{d-1}{d}}$, where τ_d stands for the kissing number of a unit ball in $\mathbb{E}^d$ (meaning the maximum number of non-overlapping unit balls of $\mathbb{E}^d$ that can touch a given unit ball in $\mathbb{E}^d$) and δ_d denotes the largest possible density for (infinite) packings of unit balls in $\mathbb{E}^d$. For further results on contact numbers, including some optimal configurations of packings of small number of unit balls in $\mathbb{E}^3$, we refer the interested reader to [2] and [17]. (See also the relevant section in [8].) On the other hand, [16] offers a focused survey on recognition-complexity results of ball contact graphs. For an overview on sphere packings we refer the interested reader to the recent books [8] and [13].

In this paper we investigate the contact numbers of finite unit ball packings that are totally separable. The notion of total separability was introduced in [11] as follows: a packing of unit balls in $\mathbb{E}^d$ is called *totally separable* if any two unit balls can be separated by a hyperplane of $\mathbb{E}^d$ such that it is disjoint from the interior of each unit ball in the packing. Finding the densest totally separable unit ball packings is a difficult problem, which is solved only in dimensions two ([11], [5]) and three ([18]). As a close combinatorial relative we want to investigate the maximum contact number $c(n, d)$ of totally separable packings of $n > 1$ unit balls in $\mathbb{E}^d, d \geq 2$. Before we state our results we make the following observation. Let $\mathbf{B}^d$ be a unit ball in an arbitrary totally separable packing of unit balls in $\mathbb{E}^d$ and assume that $\mathbf{B}^d$ is touched by m unit balls of the given packing say, at the points $\mathbf{t}_1, \dots, \mathbf{t}_m \in \mathbb{S}^{d-1}$, where the boundary of $\mathbf{B}^d$ is identified with the $(d-1)$-dimensional spherical space $\mathbb{S}^{d-1}$. The total separability of the given packing implies in a straightforward way that the spherical distance between any two points of $\{\mathbf{t}_1, \dots, \mathbf{t}_m\}$ is at least $\frac{\pi}{2}$. Now,

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recall that according to [10] (see also [19] and [22]) the maximum cardinality of a point set in $\mathbb{S}^{d-1}$ having pairwise spherical distances at least $\frac{\pi}{2}$, is $2d$ and that maximum is attained only for the vertices of a regular d-dimensional crosspolytope inscribed in $\mathbf{B}^d$. Thus, $m \leq 2d$ and therefore $c(n,d) \leq dn$. In the following we state isoperimetric-type improvements on this upper bound.

A straightforward modification of the method of Harborth [15] implies that

$$c(n,2) = \lfloor 2n - 2\sqrt{n} \rfloor \tag{1}$$

for all $n > 1$. For the convenience of the reader a proof of (1) is presented in the Appendix of this paper.

Now, let us imagine that we generate totally separable packings of unit diameter balls in $\mathbb{E}^d$ such that every center of the balls chosen, is a lattice point of the integer lattice $\mathbb{Z}^d$ in $\mathbb{E}^d$. Then let $c_{\mathbb{Z}}(n,d)$ denote the largest possible contact number of all totally separable packings of n unit diameter balls obtained in this way. It has been known for a long time ([14]) that $c_{\mathbb{Z}}(n,2) = \lfloor 2n - 2\sqrt{n} \rfloor$, which together with (1) implies that $c_{\mathbb{Z}}(n,2) = c(n,2)$ for all $n > 1$. While we do not know any explicit formula for $c_{\mathbb{Z}}(n,3)$ in terms of n, we do have the following simple asymptotic formula for $c_{\mathbb{Z}}(n,3)$ as $n \to +\infty$, which follows in a rather straightforward way from the structural-type theorem of [1] characterizing a particular extremal configuration of $c_{\mathbb{Z}}(n,3)$ for any given $n > 1$: $c_{\mathbb{Z}}(n,3) = 3n - 3n^{\frac{2}{3}} + o(n^{\frac{2}{3}})$. Clearly, $c_{\mathbb{Z}}(n,3) \leq c(n,3)$ for all $n > 1$. So, one may wonder whether $c_{\mathbb{Z}}(n,3) = c(n,3)$ for all $n > 1$?

The above discussion leads to the natural and rather basic question on upper bounding $c_{\mathbb{Z}}(n,d)$ (resp., $c(n,d)$) in the form of $dn - Cn^{\frac{d-1}{d}}$, where $C > 0$ is a proper constant depending on d.

Theorem 1. *$c_{\mathbb{Z}}(n,d) \leq \lfloor dn - dn^{\frac{d-1}{d}} \rfloor$ for all $n > 1$ and $d \geq 2$.*

We note that the upper bound of Theorem 1 is sharp for $d = 2$ and all $n > 1$ and for $d \geq 3$ and all $n = k^d$ with $k > 1$. On the other hand, it is not a sharp estimate for example, for $d = 3$ and $n = 5$.

Theorem 2. *$c(n,d) \leq \left\lfloor dn - \frac{1}{2d^{\frac{d-1}{2}}} n^{\frac{d-1}{d}} \right\rfloor$ for all $n > 1$ and $d \geq 4$.*

Although the method of the proof of Theorem 2 can be extended to include the case $d = 3$ the following statement is a stronger result.

Theorem 3. *$c(n,3) < \lfloor 3n - 1.346 n^{\frac{2}{3}} \rfloor$ for all $n > 1$.*

In the rest of the paper we prove the theorems stated.

2 Proof of Theorem 1

A union of finitely many axes parallel d-dimensional orthogonal boxes having pairwise disjoint interiors in $\mathbb{E}^d$ is called a *box-polytope*. One may call the following statement the isoperimetric inequality for box-polytopes, which together with its proof presented below is an analogue of the isoperimetric inequality for convex bodies derived from the Brunn–Minkowski inequality. (For more details on the latter see for example, [3].)

Lemma 1. *Among box-polytopes of given volume the cubes have the least surface volume.*

Proof. Without loss of generality we may assume that the volume $\mathrm{vol}_d(\mathbf{A})$ of the given box-polytope $\mathbf{A}$ in $\mathbb{E}^d$ is equal to 2^d, i.e., $\mathrm{vol}_d(\mathbf{A}) = 2^d$. Let $\mathbf{B}$ be an axes parallel d-dimensional cube of $\mathbb{E}^d$ with $\mathrm{vol}_d(\mathbf{B}) = 2^d$. Let the surface volume of $\mathbf{B}$ be denoted by $\mathrm{svol}_{d-1}(\mathbf{B})$. Clearly, $\mathrm{svol}_{d-1}(\mathbf{B}) = d \cdot \mathrm{vol}_d(\mathbf{B})$. On the other hand, if $\mathrm{svol}_{d-1}(\mathbf{A})$ denotes the surface volume of the box-polytope $\mathbf{A}$, then via the Minkowski definiton of surface volume one obtains that

$$\mathrm{svol}_{d-1}(\mathbf{A}) = \lim_{\epsilon \to 0^+} \frac{\mathrm{vol}_d(\mathbf{A} + \epsilon \mathbf{B}) - \mathrm{vol}_d(\mathbf{A})}{\epsilon} \ ,$$

where "+" in the numerator stands for the Minkowski addition of the given sets. Using the Brunn–Minkowski inequality ([3]) we get that

$$\mathrm{vol}_d(\mathbf{A}+\epsilon\mathbf{B}) \geq \left(\mathrm{vol}_d(\mathbf{A})^{\frac{1}{d}} + \mathrm{vol}_d(\epsilon\mathbf{B})^{\frac{1}{d}}\right)^d = \left(\mathrm{vol}_d(\mathbf{A})^{\frac{1}{d}} + \epsilon\cdot\mathrm{vol}_d(\mathbf{B})^{\frac{1}{d}}\right)^d .$$

Hence,

$$\mathrm{vol}_d(\mathbf{A}+\epsilon\mathbf{B}) \geq \mathrm{vol}_d(\mathbf{A}) + d\cdot\mathrm{vol}_d(\mathbf{A})^{\frac{d-1}{d}}\cdot\epsilon\cdot\mathrm{vol}_d(\mathbf{B})^{\frac{1}{d}} = \mathrm{vol}_d(\mathbf{A}) + \epsilon\cdot d\cdot\mathrm{vol}_d(\mathbf{B}) = \mathrm{vol}_d(\mathbf{A}) + \epsilon\cdot\mathrm{svol}_{d-1}(\mathbf{B}) .$$

So

$$\frac{\mathrm{vol}_d(\mathbf{A}+\epsilon\mathbf{B}) - \mathrm{vol}_d(\mathbf{A})}{\epsilon} \geq \mathrm{svol}_{d-1}(\mathbf{B})$$

and therefore $\mathrm{svol}_{d-1}(\mathbf{A}) \geq \mathrm{svol}_{d-1}(\mathbf{B})$, finishing the proof of Lemma 1. □

Corollary 1. *For any box-polytope $\mathbf{P}$ of $\mathbb{E}^d$ the isoperimetric quotient $\frac{\mathrm{svol}_{d-1}(\mathbf{P})^d}{\mathrm{vol}_d(\mathbf{P})^{d-1}}$ of $\mathbf{P}$ is at least as large as the isoperimetric quotient of a cube, i.e.,*

$$\frac{\mathrm{svol}_{d-1}(\mathbf{P})^d}{\mathrm{vol}_d(\mathbf{P})^{d-1}} \geq (2d)^d .$$

Now, let $\mathcal{P} := \{\mathbf{c}_1+\mathbf{B}^d, \mathbf{c}_2+\mathbf{B}^d, \ldots, \mathbf{c}_n+\mathbf{B}^d\}$ denote the totally separable packing of n unit diameter balls with centers $\{\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_n\} \subset \mathbb{Z}^d$ having contact number $c_{\mathbb{Z}}(n,d)$ in $\mathbb{E}^d$. ($\mathcal{P}$ might not be uniquely determined up to congruence in which case $\mathcal{P}$ stands for any of those extremal packings.) Let $\mathbf{U}^d$ be the axes parallel d-dimensional unit cube centered at the origin $\mathbf{o}$ in $\mathbb{E}^d$. Then the unit cubes $\{\mathbf{c}_1+\mathbf{U}^d, \mathbf{c}_2+\mathbf{U}^d, \ldots, \mathbf{c}_n+\mathbf{U}^d\}$ have pairwise disjoint interiors and $\mathbf{P} = \cup_{i=1}^n(\mathbf{c}_i+\mathbf{U}^d)$ is a box-polytope. Clearly, $\mathrm{svol}_{d-1}(\mathbf{P}) = 2dn - 2c_{\mathbb{Z}}(n,d)$. Hence, Corollary 1 implies that

$$2dn - 2c_{\mathbb{Z}}(n,d) = \mathrm{svol}_{d-1}(\mathbf{P}) \geq 2d\,\mathrm{vol}_d(\mathbf{P})^{\frac{d-1}{d}} = 2dn^{\frac{d-1}{d}} .$$

So, $dn - dn^{\frac{d-1}{d}} \geq c_{\mathbb{Z}}(n,d)$, finishing the proof of Theorem 1.

3 Proof of Theorem 2

Definition 1. *Let $\mathbf{B}^d = \{\mathbf{x}\in\mathbb{E}^d \mid \|\mathbf{x}\| \leq 1\}$ be the closed unit ball centered at the origin $\mathbf{o}$ in $\mathbb{E}^d$, where $\|\cdot\|$ refers to the standard Euclidean norm of $\mathbb{E}^d$. Let $R \geq 1$. We say that the packing*

$$\mathcal{P}_{\mathrm{sep}} = \{\mathbf{c}_i+\mathbf{B}^d \mid i\in I \text{ with } \|\mathbf{c}_j-\mathbf{c}_k\| \geq 2 \text{ for all } j\neq k\in I\}$$

*of (finitely or infinitely many) non-overlapping translates of $\mathbf{B}^d$ with centers $\{\mathbf{c}_i \mid i\in I\}$ is an R-*separable packing *in $\mathbb{E}^d$ if for each $i\in I$ the finite packing $\{\mathbf{c}_j+\mathbf{B}^d \mid \mathbf{c}_j+\mathbf{B}^d \subseteq \mathbf{c}_i+R\mathbf{B}^d\}$ is a totally separable packing (in $\mathbf{c}_i+R\mathbf{B}^d$). Finally, let $\delta_{\mathrm{sep}}(R,d)$ denote the largest density of all R-separable unit ball packings in $\mathbb{E}^d$, i.e., let*

$$\delta_{\mathrm{sep}}(R,d) = \sup_{\mathcal{P}_{\mathrm{sep}}}\left(\limsup_{\lambda\to\infty}\frac{\sum_{\mathbf{c}_i+\mathbf{B}^d\subset\mathbf{Q}_\lambda}\mathrm{vol}_d(\mathbf{c}_i+\mathbf{B}^d)}{\mathrm{vol}_d(\mathbf{Q}_\lambda)}\right) ,$$

where $\mathbf{Q}_\lambda$ denotes the d-dimensional cube of edge length 2λ centered at $\mathbf{o}$ in $\mathbb{E}^d$ having edges parallel to the coordinate axes of $\mathbb{E}^d$.

Remark 1. *For any $1 \leq R < 3$ we have that $\delta_{\mathrm{sep}}(R,d) = \delta_d$, where δ_d stands for the supremum of the upper densities of all unit ball packings in $\mathbb{E}^d$.*

The following statement is the core part of our proof of Theorem 2 and it is an analogue of the Lemma in [6] (see also Theorem 3.1 in [4]).

Theorem 4. *If $\{\mathbf{c}_i + \mathbf{B}^d \mid 1 \leq i \leq n\}$ is an R-separable packing of n unit balls in $\mathbb{E}^d$ with $R \geq 1$, $n \geq 1$, and $d \geq 2$, then*

$$\frac{n\mathrm{vol}_d(\mathbf{B}^d)}{\mathrm{vol}_d\left(\cup_{i=1}^n \mathbf{c}_i + 2R\mathbf{B}^d\right)} \leq \delta_{\mathrm{sep}}(R,d) \ .$$

Proof. Assume that the claim is not true. Then there is an $\epsilon > 0$ such that

$$\mathrm{vol}_d\left(\cup_{i=1}^n \mathbf{c}_i + 2R\mathbf{B}^d\right) = \frac{n\mathrm{vol}_d(\mathbf{B}^d)}{\delta_{\mathrm{sep}}(R,d)} - \epsilon \tag{2}$$

Let $C_n = \{\mathbf{c}_i \mid i = 1, \ldots, n\}$ and let Λ be a packing lattice of $C_n + 2R\mathbf{B}^d = \cup_{i=1}^n \mathbf{c}_i + 2R\mathbf{B}^d$ such that $C_n + 2R\mathbf{B}^d$ is contained in the foundamental parallelotope $\mathbf{P}$ of Λ. Recall that for each $\lambda > 0$, $\mathbf{Q}_\lambda$ denotes the d-dimensional cube of edge length 2λ centered at the origin $\mathbf{o}$ in $\mathbb{E}^d$ having edges parallel to the coordinate axes of $\mathbb{E}^d$. Clearly, there is a constant $\mu > 0$ depending on $\mathbf{P}$ only, such that for each $\lambda > 0$ there is a subset L_λ of Λ with

$$\mathbf{Q}_\lambda \subseteq L_\lambda + \mathbf{P} \text{ and } L_\lambda + 2\mathbf{P} \subseteq \mathbf{Q}_{\lambda+\mu} \ . \tag{3}$$

Moreover, let $\mathcal{P}_m(\mathbf{B}^d)$ denote the family of all R-separable packings of $m > 1$ unit balls in $\mathbb{E}^d$. The definition of $\delta_{\mathrm{sep}}(R,d)$ implies that for each $\lambda > 0$ there exists a packing in the family $\mathcal{P}_m(\mathbf{B}^d)$ with centers at the points of $C_{m(\lambda)}$ such that

$$C_{m(\lambda)} + \mathbf{B}^d \subset \mathbf{Q}_\lambda$$

and

$$\lim_{\lambda\to\infty} \frac{m(\lambda)\mathrm{vol}_d(\mathbf{B}^d)}{\mathrm{vol}_d(\mathbf{Q}_\lambda)} = \delta_{\mathrm{sep}}(R,d) \ .$$

As $\lim_{\lambda\to\infty} \frac{\mathrm{vol}_d(\mathbf{Q}_{\lambda+\mu})}{\mathrm{vol}_d(\mathbf{Q}_\lambda)} = 1$ therefore there exist $\xi > 0$ and a packing in the family $\mathcal{P}_{m(\xi)}(\mathbf{B}^d)$ with centers at the points of $C_{m(\xi)}$ and with $C_{m(\xi)} + \mathbf{B}^d \subset \mathbf{Q}_\xi$ such that

$$\frac{\mathrm{vol}_d(\mathbf{P})\delta_{\mathrm{sep}}(R,d)}{\mathrm{vol}_d(\mathbf{P}) + \epsilon} < \frac{m(\xi)\mathrm{vol}_d(\mathbf{B}^d)}{\mathrm{vol}_d(\mathbf{Q}_{\xi+\mu})} \text{ and } \frac{n\mathrm{vol}_d(\mathbf{B}^d)}{\mathrm{vol}_d(\mathbf{P}) + \epsilon} < \frac{n\mathrm{vol}_d(\mathbf{B}^d)\mathrm{card}(L_\xi)}{\mathrm{vol}_d(\mathbf{Q}_{\xi+\mu})} \ , \tag{4}$$

where $\mathrm{card}(\cdot)$ refers to the cardinality of the given set. Now, for each $\mathbf{x} \in \mathbf{P}$ we define an R-separable packing of $n(\mathbf{x})$ translates of $\mathbf{B}^d$ in $\mathbb{E}^d$ with centers at the points of

$$C_{n(\mathbf{x})} = \{\mathbf{x} + L_\xi + C_n\} \cup \{\mathbf{y} \in C_{m(\xi)} \mid \mathbf{y} \notin \mathbf{x} + L_\xi + C_n + \mathrm{int}(2R\mathbf{B}^d)\} \ ,$$

where $\mathrm{int}(\cdot)$ refers to the interior of the given set in $\mathbb{E}^d$. Clearly, (3) implies that $C_{n(\mathbf{x})} + \mathbf{B}^d \subset \mathbf{Q}_{\xi+\mu}$. Now, in order to evaluate $\int_{\mathbf{x}\in\mathbf{P}} n(\mathbf{x})d\mathbf{x}$, we introduce the function $\chi_\mathbf{y}$ for each $\mathbf{y} \in C_{m(\xi)}$ defined as follows: $\chi_\mathbf{y}(\mathbf{x}) = 1$ if $\mathbf{y} \notin \mathbf{x} + L_\xi + C_n + \mathrm{int}(2R\mathbf{B}^d)$ and $\chi_\mathbf{y}(\mathbf{x}) = 0$ for any other $\mathbf{x} \in \mathbf{P}$. Then it is easy to see that

$$\int_{\mathbf{x}\in\mathbf{P}} n(\mathbf{x})d\mathbf{x} = \int_{\mathbf{x}\in\mathbf{P}} \big(n\mathrm{card}(L_\xi) + \sum_{\mathbf{y}\in C_{m(\xi)}} \chi_\mathbf{y}(\mathbf{x})\big)d\mathbf{x} = n\mathrm{vol}_d(\mathbf{P})\mathrm{card}(L_\xi) + m(\xi)\big(\mathrm{vol}_d(\mathbf{P}) - \mathrm{vol}_d(C_n + 2R\mathbf{B}^d)\big) \ .$$

Hence, there is a point $\mathbf{p} \in \mathbf{P}$ with

$$n(\mathbf{p}) \geq m(\xi)\left(1 - \frac{\mathrm{vol}_d(C_n + 2R\mathbf{B}^d)}{\mathrm{vol}_d(\mathbf{P})}\right) + n\mathrm{card}(L_\xi)$$

and so

$$\frac{n(\mathbf{p})\mathrm{vol}_d(\mathbf{B}^d)}{\mathrm{vol}_d(\mathbf{Q}_{\xi+\mu})} \geq \frac{m(\xi)\mathrm{vol}_d(\mathbf{B}^d)}{\mathrm{vol}_d(\mathbf{Q}_{\xi+\mu})}\left(1 - \frac{\mathrm{vol}_d(C_n + 2R\mathbf{B}^d)}{\mathrm{vol}_d(\mathbf{P})}\right) + \frac{n\mathrm{vol}_d(\mathbf{B}^d)\mathrm{card}(L_\xi)}{\mathrm{vol}_d(\mathbf{Q}_{\xi+\mu})} \ . \tag{5}$$

Now, (2) implies in a straightforward way that

$$\frac{\mathrm{vol}_d(\mathbf{P})\delta_{\mathrm{sep}}(R,d)}{\mathrm{vol}_d(\mathbf{P}) + \epsilon}\left(1 - \frac{\mathrm{vol}_d(C_n + 2R\mathbf{B}^d)}{\mathrm{vol}_d(\mathbf{P})}\right) + \frac{n\mathrm{vol}_d(\mathbf{B}^d)}{\mathrm{vol}_d(\mathbf{P}) + \epsilon} = \delta_{\mathrm{sep}}(R,d) \tag{6}$$

Thus, (4), (5), and (6) yield that

$$\frac{n(\mathbf{p})\mathrm{vol}_d(\mathbf{B}^d)}{\mathrm{vol}_d(\mathbf{Q}_{\xi+\mu})} > \delta_{\mathrm{sep}}(R,d)\ .$$

As $C_{n(\mathbf{p})}+\mathbf{B}^d\subset\mathbf{Q}_{\xi+\mu}$ this contradicts the definition of $\delta_{\mathrm{sep}}(R,d)$, finishing the proof of Theorem 4. $\square$

Next, let $\mathcal{P}=\{\mathbf{c}_1+\mathbf{B}^d,\mathbf{c}_2+\mathbf{B}^d,\dots,\mathbf{c}_n+\mathbf{B}^d\}$ be a totally separable packing of n translates of $\mathbf{B}^d$ with centers at the points of $C_n=\{\mathbf{c}_1,\mathbf{c}_2,\dots,\mathbf{c}_n\}$ in $\mathbb{E}^d$. Recall that any member of $\mathcal{P}$ is tangent to at most $2d$ members of $\mathcal{P}$ and if $\mathbf{c}_i+\mathbf{B}^d$ is tangent to $2d$ members, then the tangent points are the vertices of a regular cross-polytope inscribed in $\mathbf{c}_i+\mathbf{B}^d$ and therefore

$$\mathbf{c}_i+\sqrt{d}\mathbf{B}^d\subset\bigcup_{1\le j\le n, j\neq i}\mathbf{c}_j+\sqrt{d}\mathbf{B}^d\ .$$

Thus, if m denotes the number of members of $\mathcal{P}$ that are tangent to $2d$ members in $\mathcal{P}$, then the $(d-1)$-dimensional surface volume $\mathrm{svol}_{d-1}\left(\mathrm{bd}(C_n+\sqrt{d}\mathbf{B}^d)\right)$ of the boundary $\mathrm{bd}(C_n+\sqrt{d}\mathbf{B}^d)$ of the non-convex set $C_n+\sqrt{d}\mathbf{B}^d$ must satisfy the inequality

$$\mathrm{svol}_{d-1}\left(\mathrm{bd}(C_n+\sqrt{d}\mathbf{B}^d)\right)\le(n-m)d^{\frac{d-1}{2}}\mathrm{svol}_{d-1}\left(\mathrm{bd}(\mathbf{B}^d)\right) \tag{7}$$

Finally, the isoperimetric inequality ([21]) applied to $C_n+\sqrt{d}\mathbf{B}^d$ yields

$$\mathrm{Iq}(\mathbf{B}^d)=\frac{\mathrm{svol}_{d-1}\left(\mathrm{bd}(\mathbf{B}^d)\right)^d}{\mathrm{vol}_d(\mathbf{B}^d)^{d-1}}=d^d\mathrm{vol}_d(\mathbf{B}^d)\le\mathrm{Iq}(C_n+\sqrt{d}\mathbf{B}^d)=\frac{\mathrm{svol}_{d-1}\left(\mathrm{bd}(C_n+\sqrt{d}\mathbf{B}^d)\right)^d}{\mathrm{vol}_d(C_n+\sqrt{d}\mathbf{B}^d)^{d-1}}\ , \tag{8}$$

where $\mathrm{Iq}(\cdot)$ stands for the isoperimetric quotient of the given set. As $d\ge4$, $\mathcal{P}$ is a $\frac{\sqrt{d}}{2}$-separable packing (in fact, it is an R-separable packing for all $R\ge1$) and therefore (7), (8), and Theorem 4 imply in a straightforward way that

$$n-m\ge\frac{\mathrm{svol}_{d-1}\left(\mathrm{bd}(C_n+\sqrt{d}\mathbf{B}^d)\right)}{d^{\frac{d-1}{2}}\mathrm{svol}_{d-1}\left(\mathrm{bd}(\mathbf{B}^d)\right)}=\frac{\mathrm{svol}_{d-1}\left(\mathrm{bd}(C_n+\sqrt{d}\mathbf{B}^d)\right)}{d^{\frac{d+1}{2}}\mathrm{vol}_d(\mathbf{B}^d)}\ge\frac{\mathrm{Iq}(\mathbf{B}^d)^{\frac{1}{d}}\mathrm{vol}_d(C_n+\sqrt{d}\mathbf{B}^d)^{\frac{d-1}{d}}}{d^{\frac{d+1}{2}}\mathrm{vol}_d(\mathbf{B}^d)}$$

$$\ge\frac{\mathrm{Iq}(\mathbf{B}^d)^{\frac{1}{d}}}{d^{\frac{d+1}{2}}\mathrm{vol}_d(\mathbf{B}^d)}\left(\frac{n\mathrm{vol}_d(\mathbf{B}^d)}{\delta_{\mathrm{sep}}(\frac{\sqrt{d}}{2},d)}\right)^{\frac{d-1}{d}}=\frac{1}{d^{\frac{d-1}{2}}\delta_{\mathrm{sep}}(\frac{\sqrt{d}}{2},d)^{\frac{d-1}{d}}}n^{\frac{d-1}{d}}\ .$$

Thus, the number of contacts in $\mathcal{P}$ is at most

$$\frac{1}{2}\left(2dn-(n-m)\right)\le dn-\frac{1}{2d^{\frac{d-1}{2}}\delta_{\mathrm{sep}}(\frac{\sqrt{d}}{2},d)^{\frac{d-1}{d}}}n^{\frac{d-1}{d}}<dn-\frac{1}{2d^{\frac{d-1}{2}}}n^{\frac{d-1}{d}}\ ,$$

finishing the proof of Theorem 2.

4 Proof of Theorem 3

The following proof is an analogue of the proof of Theorem 1.1 in [7] and as such it is based on the proper modifications of the main (resp., technical) lemmas of [7]. Overall the method discussed below turns out to be more efficient for totally separable unit ball packings than for unit ball packings in general. The more exact details are as follows.

Let $\mathbf{B}^3$ denote the (closed) unit ball centered at the origin $\mathbf{o}$ of $\mathbb{E}^3$ and let $\mathcal{P}:=\{\mathbf{c}_1+\mathbf{B}^3,\mathbf{c}_2+\mathbf{B}^3,\dots,\mathbf{c}_n+\mathbf{B}^3\}$ denote the totally separable packing of n unit balls with centers $\mathbf{c}_1,\mathbf{c}_2,\dots,\mathbf{c}_n$ in $\mathbb{E}^3$, which has the largest number namely, $c(n,3)$ of touching pairs among all totally separable packings of n unit balls in $\mathbb{E}^3$. ($\mathcal{P}$ might not be uniquely determined up to congruence in which case $\mathcal{P}$ stands for any of those extremal packings.)

Lemma 2.
$$\frac{\frac{4\pi}{3}n}{\mathrm{vol}_3\left(\bigcup_{i=1}^{n}\left(\mathbf{c}_i+\sqrt{3}\mathbf{B}^3\right)\right)}<0.6401,$$
where $\mathrm{vol}_3(\cdot)$ *refers to the* 3*-dimensional volume of the corresponding set.*

Proof. First, partition $\bigcup_{i=1}^{n}\left(\mathbf{c}_i+\sqrt{3}\mathbf{B}^3\right)$ into truncated Voronoi cells as follows. Let $\mathbf{P}_i$ denote the Voronoi cell of the packing $\mathcal{P}$ assigned to $\mathbf{c}_i+\mathbf{B}^3$, $1\leq i\leq n$, that is, let $\mathbf{P}_i$ stand for the set of points of $\mathbb{E}^3$ that are not farther away from $\mathbf{c}_i$ than from any other $\mathbf{c}_j$ with $j\neq i, 1\leq j\leq n$. Then, recall the well-known fact (see for example, [12]) that the Voronoi cells $\mathbf{P}_i$, $1\leq i\leq n$ just introduced form a tiling of $\mathbb{E}^3$. Based on this it is easy to see that the truncated Voronoi cells $\mathbf{P}_i\cap(\mathbf{c}_i+\sqrt{3}\mathbf{B}^3)$, $1\leq i\leq n$ generate a tiling of the non-convex container $\bigcup_{i=1}^{n}\left(\mathbf{c}_i+\sqrt{3}\mathbf{B}^3\right)$ for the packing $\mathcal{P}$. Second, we prove the following metric properties of the Voronoi cells introduced above.

Sublemma 1. *The distance between the line of an arbitrary edge of the Voronoi cell* $\mathbf{P}_i$ *and the center* $\mathbf{c}_i$ *is always at least* $\frac{3\sqrt{3}}{4}=1.299\ldots$ *for any* $1\leq i\leq n$*.*

Proof. It is easy to see that the claim follows from the following 2-dimensional statement: If $\{\mathbf{a}+\mathbf{B}^2,\mathbf{b}+\mathbf{B}^2,\mathbf{c}+\mathbf{B}^2\}$ is a totally separable packing of three unit disks with centers $\mathbf{a},\mathbf{b},\mathbf{c}$ in $\mathbb{E}^2$, then the circumradius of the triangle $\triangle\mathbf{abc}$ is at least $\frac{3\sqrt{3}}{4}$. An easy argument implies that in order to prove the latter claim it is sufficient to check it for triangles $\mathbf{abc}$ with the property that the two inner tangent lines of the unit disks $\mathbf{a}+\mathbf{B}^2$ and $\mathbf{b}+\mathbf{B}^2$ are tangent to the unit disk $\mathbf{c}+\mathbf{B}^2$ as well. Furthermore, one can assume that $2<\|\mathbf{a}-\mathbf{b}\|\leq 2\sqrt{2}$ and $2<\|\mathbf{a}-\mathbf{c}\|=\|\mathbf{b}-\mathbf{c}\|\leq 2\sqrt{2}$. Now, if $x=\frac{1}{2}\|\mathbf{a}-\mathbf{b}\|$, then an elementary computation yields that the circumradius of the triangle $\mathbf{abc}$ is equal to $f(x)=\frac{x^3}{2\sqrt{x^2-1}}$ with $1<x\leq\sqrt{2}$. Finally, $f'(x)=\frac{x^2(2x^2-3)}{2(x^2-1)\sqrt{x^2-1}}$ implies in a straightforward way that $f(\sqrt{\frac{3}{2}})=\frac{3\sqrt{3}}{4}$ is a global minimum of $f(x)$ over $1<x\leq\sqrt{2}$. This finishes the proof of Sublemma 1. □

Remark 2. *As one can see from the above proof, the lower bound of Sublemma 1 is a sharp one and it should be compared to the lower bound* $\frac{2}{\sqrt{3}}=1.154\ldots$ *valid for any unit ball packing not necessarily totally separable in* $\mathbb{E}^3$*. (For more details on the lower bound* $\frac{2}{\sqrt{3}}$ *see for example the discussion on page 29 in [8].)*

Sublemma 2. *The distance between an arbitrary vertex of the Voronoi cell* $\mathbf{P}_i$ *and the center* $\mathbf{c}_i$ *is always at least* $\sqrt{2}=1.414\ldots$ *for any* $1\leq i\leq n$*.*

Proof. Clearly, the claim follows from the following statement: If $\mathcal{P}_4=\{\mathbf{c}_1+\mathbf{B}^3,\mathbf{c}_2+\mathbf{B}^3,\mathbf{c}_3+\mathbf{B}^3,\mathbf{c}_4+\mathbf{B}^3\}$ is a totally separable packing of four unit balls with centers $\mathbf{c}_1,\mathbf{c}_2,\mathbf{c}_3,\mathbf{c}_4$ in $\mathbb{E}^3$, then the circumradius of the terahedron $\mathbf{c}_1\mathbf{c}_2\mathbf{c}_3\mathbf{c}_4$ is at least $\sqrt{2}$. We prove the latter claim by looking at the following two cases possible. $\mathcal{P}_4$ is a totally separable packing with plane H separating either $\mathbf{c}_1+\mathbf{B}^3,\mathbf{c}_2+\mathbf{B}^3$ from $\mathbf{c}_3+\mathbf{B}^3,\mathbf{c}_4+\mathbf{B}^3$ (*Case 1*) or $\mathbf{c}_1+\mathbf{B}^3$ from $\mathbf{c}_2+\mathbf{B}^3,\mathbf{c}_3+\mathbf{B}^3,\mathbf{c}_4+\mathbf{B}^3$ (*Case 2*). In both cases it is sufficient to show that if $\cup_{i=1}^{4}\mathbf{c}_i+\mathbf{B}^3\subset\mathbf{x}+r\mathbf{B}^3$ for some $\mathbf{x}\in\mathbb{E}^3$ and $r\in\mathbb{R}$, then $r\geq 1+\sqrt{2}$.
Case 1: Let H^+ and H^- denote the two closed halfspaces bounded by H with $\mathbf{c}_1+\mathbf{B}^3\cup\mathbf{c}_2+\mathbf{B}^3\subset H^+$ and $\mathbf{c}_3+\mathbf{B}^3\cup\mathbf{c}_4+\mathbf{B}^3\subset H^-$. Without loss of generality we may assume that $\mathrm{vol}_3\left((\mathbf{x}+r\mathbf{B}^3)\cap H^+\right)\leq\mathrm{vol}_3\left((\mathbf{x}+r\mathbf{B}^3)\cap H^-\right)$. Now, if $\mathbf{c}'_1$ (resp., $\mathbf{c}'_2$) denotes the image of $\mathbf{c}_1$ (resp., $\mathbf{c}_2$) under the reflection about H, then clearly $\mathcal{P}'=\{\mathbf{c}_1+\mathbf{B}^3,\mathbf{c}_2+\mathbf{B}^3,\mathbf{c}'_1+\mathbf{B}^3,\mathbf{c}'_2+\mathbf{B}^3\}$ is a packing of four unit balls in $\mathbf{x}+r\mathbf{B}^3$ symmetric about H. Then using the symmetry of $\mathcal{P}'$ with respect to H it is easy to see that $r\geq 1+\sqrt{2}$.
Case 2: Let H^+ and H^- denote the two closed halfspaces bounded by H with $\mathbf{c}_1+\mathbf{B}^3\subset H^+$ and $\mathbf{c}_2+\mathbf{B}^3\cup\mathbf{c}_3+\mathbf{B}^3\cup\mathbf{c}_4+\mathbf{B}^3\subset H^-$. If one assumes that $r-1<\sqrt{2}$, then using $\mathbf{c}_1\in(\mathbf{x}+(r-1)\mathbf{B}^3)\cap H^+$ and $\{\mathbf{c}_2,\mathbf{c}_3,\mathbf{c}_4\}\subset(\mathbf{x}+(r-1)\mathbf{B}^3)\cap H^-$ it is easy to see that the triangle $\mathbf{c}_2\mathbf{c}_3\mathbf{c}_4$ is contained in a disk of radius less than $2\sqrt{\sqrt{2}-1}=1.287\ldots$. On the other hand, as the unit balls $\mathbf{c}_2+\mathbf{B}^3,\mathbf{c}_3+\mathbf{B}^3,\mathbf{c}_4+\mathbf{B}^3$ form a totally separable packing therefore the proof of Sublemma 1 implies that the radius of any disk containing the triangle $\mathbf{c}_2\mathbf{c}_3\mathbf{c}_4$ must be at least $\frac{3\sqrt{3}}{4}=1.299\ldots$, a contradiction. □

Remark 3. *As one can see from the above proof, the lower bound of Sublemma 2 is a sharp one and it should be compared to the lower bound* $\sqrt{\frac{3}{2}} = 1.224\ldots$ *valid for any unit ball packing not necessarily totally separable in* $\mathbb{E}^3$. *(For more details on the lower bound* $\sqrt{\frac{3}{2}}$ *see for example the discussion on page 29 in [8].)*

Now, let $\mathbf{U} := \mathrm{conv}(\{\mathbf{o}, \mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3\})$ be the following special tetrahedron, also called the orthoscheme with vertices $\mathbf{o}, \mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3$ in $\mathbb{E}^3$ (where $\mathrm{conv}(\cdot)$ refers to the convex hull of the given set): $\mathbf{u}_1$ is orthogonal to $\mathbf{u}_2 - \mathbf{u}_1$ as well as $\mathbf{u}_3 - \mathbf{u}_1$, and $\mathbf{u}_2$ is orthogonal to $\mathbf{u}_3 - \mathbf{u}_2$ moreover, $\|\mathbf{u}_1\| = 1$, $\|\mathbf{u}_2\| = \frac{3\sqrt{3}}{4}$, and $\|\mathbf{u}_3\| = \sqrt{2}$ (where $\|\cdot\|$ denotes the Euclidean norm of $\mathbb{E}^3$). Rogers's well-known method ([24]) on dissecting each Voronoi cell $\mathbf{P}_i$ into special simplices called Rogers simplices combined with Sublemmas 1 and 2 imply the following estimate in a standard way (using the so-called Lemma of Comparison of Rogers (for more details see for example, page 33 in [8])).

Sublemma 3.

$$\frac{\frac{4\pi}{3}}{\mathrm{vol}_3(\mathbf{P}_i \cap (\mathbf{c}_i + \sqrt{2}\mathbf{B}^3))} \leq \frac{\mathrm{vol}_3(\mathbf{U} \cap \mathbf{B}^3)}{\mathrm{vol}_3(\mathbf{U})} < 0.6401.$$

As $\mathbf{P}_i \cap (\mathbf{c}_i + \sqrt{2}\mathbf{B}^3) \subset \mathbf{P}_i \cap (\mathbf{c}_i + \sqrt{3}\mathbf{B}^3)$, therefore Sublemma 3 completes the proof of Lemma 2. $\square$

The well-known isoperimetric inequality ([21]) applied to $\bigcup_{i=1}^{n} \left(\mathbf{c}_i + \sqrt{3}\mathbf{B}^3\right)$ yields

Lemma 3.

$$36\pi \ \mathrm{vol}_3 \left(\bigcup_{i=1}^{n} \left(\mathbf{c}_i + \sqrt{3}\mathbf{B}^3 \right) \right)^2 \leq \mathrm{svol}_2 \left(\mathrm{bd} \left(\bigcup_{i=1}^{n} \left(\mathbf{c}_i + \sqrt{3}\mathbf{B}^3 \right) \right) \right)^3,$$

where $\mathrm{svol}_2(\cdot)$ *refers to the* 2*-dimensional surface volume of the corresponding set.*

Thus, Lemma 2 and Lemma 3 generate the following inequality.

Corollary 2.

$$\frac{4\pi}{(0.6401)^{\frac{2}{3}}} n^{\frac{2}{3}} < \mathrm{svol}_2 \left(\mathrm{bd} \left(\bigcup_{i=1}^{n} \left(\mathbf{c}_i + \sqrt{3}\mathbf{B}^3 \right) \right) \right).$$

Now, assume that $\mathbf{c}_i + \mathbf{B}^3 \in \mathcal{P}$ is tangent to $\mathbf{c}_j + \mathbf{B}^3 \in \mathcal{P}$ for all $j \in T_i$, where $T_i \subset \{1, 2, \ldots, n\}$ stands for the family of indices $1 \leq j \leq n$ for which $\mathrm{dist}(\mathbf{c}_i, \mathbf{c}_j) = 2$. Then let $\hat{S}_i := \mathrm{bd}(\mathbf{c}_i + \sqrt{3}\mathbf{B})$ and let $\hat{\mathbf{c}}_{ij}$ be the intersection of the line segment $\mathbf{c}_i\mathbf{c}_j$ with $\hat{S}_i$ for all $j \in T_i$. Moreover, let $C_{\hat{S}_i}(\hat{\mathbf{c}}_{ij}, \frac{\pi}{4})$ (resp., $C_{\hat{S}_i}(\hat{\mathbf{c}}_{ij}, \alpha)$) denote the open spherical cap of $\hat{S}_i$ centered at $\hat{\mathbf{c}}_{ij} \in \hat{S}_i$ having angular radius $\frac{\pi}{4}$ (resp., α with $0 < \alpha < \frac{\pi}{2}$ and $\cos\alpha = \frac{1}{\sqrt{3}}$). As $\mathcal{P}$ is totally separable therefore the family $\{C_{\hat{S}_i}(\hat{\mathbf{c}}_{ij}, \frac{\pi}{4}), j \in T_i\}$ consists of pairwise disjoint open spherical caps of $\hat{S}_i$; moreover,

$$\frac{\sum_{j \in T_i} \mathrm{svol}_2 \left(C_{\hat{S}_i}(\hat{\mathbf{c}}_{ij}, \frac{\pi}{4}) \right)}{\mathrm{svol}_2 \left(\cup_{j \in T_i} C_{\hat{S}_i}(\hat{\mathbf{c}}_{ij}, \alpha) \right)} = \frac{\sum_{j \in T_i} \mathrm{Sarea}\left(C(\mathbf{u}_{ij}, \frac{\pi}{4}) \right)}{\mathrm{Sarea}\left(\cup_{j \in T_i} C(\mathbf{u}_{ij}, \alpha) \right)}, \tag{9}$$

where $\mathbf{u}_{ij} := \frac{1}{2}(\mathbf{c}_j - \mathbf{c}_i) \in \mathbb{S}^2 := \mathrm{bd}(\mathbf{B}^3)$ and $C(\mathbf{u}_{ij}, \frac{\pi}{4}) \subset \mathbb{S}^2$ (resp., $C(\mathbf{u}_{ij}, \alpha) \subset \mathbb{S}^2$) denotes the open spherical cap of $\mathbb{S}^2$ centered at $\mathbf{u}_{ij}$ having angular radius $\frac{\pi}{4}$ (resp., α) and where $\mathrm{Sarea}(\cdot)$ refers to the spherical area measure on $\mathbb{S}^2$.

Lemma 4.

$$\frac{\sum_{j \in T_i} \mathrm{Sarea}\left(C(\mathbf{u}_{ij}, \frac{\pi}{4}) \right)}{\mathrm{Sarea}\left(\cup_{j \in T_i} C(\mathbf{u}_{ij}, \alpha) \right)} \leq 3 \left(1 - \frac{1}{\sqrt{2}} \right) = 0.8786\ldots \ .$$

Proof. By assumption $\mathcal{P}_i(\mathbb{S}^2) = \{C(\mathbf{u}_{ij}, \frac{\pi}{4}) \mid j \in T_i\}$ is a packing of spherical caps of angular radius $\frac{\pi}{4}$ in $\mathbb{S}^2$. Let $V_{ij}(\mathbb{S}^2)$ denote the Voronoi region of the packing $\mathcal{P}_i(\mathbb{S}^2)$ assigned to $C(\mathbf{u}_{ij}, \frac{\pi}{4})$, that is, let $V_{ij}(\mathbb{S}^2)$ stand for the set of points of $\mathbb{S}^2$ that are not farther away from $\mathbf{u}_{ij}$ than from any other $\mathbf{u}_{ik}$ with $k \neq j, k \in T_i$. Recall (see for example [12]) that the Voronoi regions $V_{ij}(\mathbb{S}^2)$, $j \in T_i$ are spherically convex polygons and form a tiling of $\mathbb{S}^2$. Moreover, it is easy to see that no vertex of $V_{ij}(\mathbb{S}^2)$ belongs to the interior of $C(\mathbf{u}_{ij}, \alpha)$ in $\mathbb{S}^2$. Thus, Hajós Lemma (Hilfssatz 1 in [20]) implies that $\mathrm{Sarea}\left(V_{ij}(\mathbb{S}^2) \cap C(\mathbf{u}_{ij}, \alpha)\right) \geq \frac{2\pi}{3}$, where $\frac{2\pi}{3}$ stands for the spherical area of a regular spherical quadrilateral inscribed into $C(\mathbf{u}_{ij}, \alpha)$ with sides tangent to $C(\mathbf{u}_{ij}, \frac{\pi}{4})$. Hence,

$$\frac{\mathrm{Sarea}\left(C(\mathbf{u}_{ij}, \frac{\pi}{4})\right)}{\mathrm{Sarea}\left(V_{ij}(\mathbb{S}^2) \cap C(\mathbf{u}_{ij}, \alpha)\right)} \leq 3\left(1 - \frac{1}{\sqrt{2}}\right) . \tag{10}$$

As the truncated Voronoi regions $V_{ij}(\mathbb{S}^2) \cap C(\mathbf{u}_{ij}, \alpha)$, $j \in T_i$ form a tiling of $\cup_{j \in T_i} C(\mathbf{u}_{ij}, \alpha)$ therefore (10) finishes the proof of Lemma 4. $\square$

Lemma 4 implies in a straightforward way that

$$\mathrm{svol}_2\left(\mathrm{bd}\left(\bigcup_{i=1}^{n}\left(\mathbf{c}_i + \sqrt{3}\mathbf{B}^3\right)\right)\right) \leq 12\pi n - \frac{1}{3\left(1 - \frac{1}{\sqrt{2}}\right)} 12\pi\left(1 - \frac{1}{\sqrt{2}}\right) c(n,3) = 12\pi n - 4\pi c(n,3). \tag{11}$$

Hence, Corollary 2 and (11) yield

$$\frac{4\pi}{(0.6401)^{\frac{2}{3}}} n^{\frac{2}{3}} < 12\pi n - 4\pi c(n,3),$$

from which it follows that $c(n,3) < 3n - \frac{1}{(0.6401)^{\frac{2}{3}}} n^{\frac{2}{3}} < 3n - 1.346 n^{\frac{2}{3}}$, finishing the proof of Theorem 3.

5 Appendix

We use the method of Harborth [15] with some natural modifications due to the total separability of the packings under investigation. We prove (1) by induction on n. For simplicity let $c(n) := c(n,2)$. Clearly, $c(2) = 1 = \lfloor 2 \cdot 2 - 2\sqrt{2} \rfloor$. So in what follows, we assume that $n \geq 3$ and in particular, we assume that (1) holds for all positive integers n' with $2 \leq n' \leq n-1$. Let $\mathcal{P}_n$ be the totally separable packing of n unit disks in $\mathbb{E}^2$, which has the largest number namely, $c(n)$ of touching pairs among all totally separable packings of n unit disks in $\mathbb{E}^2$. ($\mathcal{P}_n$ might not be uniquely determined up to congruence in which case $\mathcal{P}_n$ stands for any of those extremal packings.) Let G_n denote the embedded contact graph of $\mathcal{P}_n$ with vertices identical to the centers of the unit disks in $\mathcal{P}_n$ and with edges represented by line segments connecting two vertices if the unit disks centered at them touch each other. Clearly, the number of edges of G_n is equal to $c(n)$. As $c(n-1)+1 = \lfloor 2(n-1) - 2\sqrt{n-1} \rfloor + 1 \leq \lfloor 2n - 2\sqrt{n} \rfloor$ and $c_{\mathbb{Z}}(n,2) = \lfloor 2n - 2\sqrt{n} \rfloor$ ([14]) for all $n \geq 2$, therefore one can assume that every vertex of G_n is adjacent to at least two other vertices (otherwise there is a vertex of G_n of degree one and so, the proof is finished by induction). In addition, using $c_{\mathbb{Z}}(n,2) = \lfloor 2n - 2\sqrt{n} \rfloor$ again one can assume that G_n is 2-connected, that is, G_n remains connected after the removal of any of its vertices.

Thus, the outer face of G_n in $\mathbb{E}^2$ is bounded by a simple closed polygon P. Let b denote the number of vertices of P. As $\mathcal{P}_n$ is a totally separable unit disk packing therefore the degree of any vertex of P (resp., G_n) is either 2 or 3 or 4 in G_n. Let b_i stand for the number of vertices of P of degree i with $2 \leq i \leq 4$. Clearly, $b = b_2 + b_3 + b_4$. Due to the total separability of $\mathcal{P}_n$, the internal angle of P at a vertex of degree i is at least $\frac{(i-1)\pi}{2}$, and the sum of these angles is $(b-2)\pi$. Thus,

$$b_2 + 2b_3 + 3b_4 \leq 2b - 4 \tag{12}$$

Next, let f_i denote the number of internal faces of G_n having i sides. As $\mathcal{P}_n$ is totally separable therefore $i \geq 4$. Now, Euler's formula implies that

$$n - c(n) + f_4 + f_5 + \ldots = 1 \tag{13}$$

If we add up the number of sides of the internal faces of G_n, then every edge of P is counted once and all the other edges twice. Thus,

$$4(f_4 + f_5 + \ldots) \leq 4f_4 + 5f_5 + \ldots = b + 2(c(n) - b). \tag{14}$$

Clearly, (13) and (14) imply that $4(1 - n + c(n)) \leq b + 2(c(n) - b)$ and so,

$$2c(n) - 3n + 4 \leq n - b \tag{15}$$

Now, let us delete from G_n the vertices of P together with the edges incident to them. By the definition of $c(n-b)$, one obtains

$$c(n) - b - (b_3 + 2b_4) \leq c(n-b). \tag{16}$$

Next, (12) and (16) imply

$$c(n) \leq c(n-b) + 2b - 4. \tag{17}$$

As by induction $c(n-b) \leq 2(n-b) - 2\sqrt{n-b}$, therefore (17) yields

$$c(n) \leq (2n-4) - 2\sqrt{n-b}. \tag{18}$$

Finally, (15) and (18) imply $c(n) \leq (2n-4) - 2\sqrt{2c(n) - 3n + 4}$, from which it follows easily that

$$0 \leq c(n)^2 - 4nc(n) + (4n^2 - 4n). \tag{19}$$

Notice that the roots of the quadratic equation $0 = x^2 - 4nx + (4n^2 - 4n)$ are $2n \pm 2\sqrt{n}$. As $c(n) < 2n$, therefore (19) implies in a straightforward way that $c(n) \leq 2n - 2\sqrt{n}$, finishing the proof of (1).

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